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AN ANALYTICAL AIR POLLUTION MODEL FOR WARM SOURCES

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Abstract. *In this work we present the GILTT method for the solution of the transient two-dimensional advection-diffusion equation incorporating the plume rise effect (warm source) using the approach proposed by Briggs (1975). A correct estimation of buoyant plume rise is one of the basic requirements for the determination of ground-level concentrations of airborne pollutant emitted by industrial stacks. This improvement turns out a more operative model. To investigate the performances of the model with the plume rise effect, we report numerical simulations of the ground-leve centerline concentrations compared with the observed concentrations measured during the Kinkaid experiment.*

Keywords*: GILTT, Analytical Solution, Advection-Diffusion equation, Atmospheric Dispersion, Warm Sources.*

1. Introduction

Eulerian approach for modelling the statistical properties of the concentrations of contaminants in a turbulent flow as the Planetary Boundary Layer (PBL) is widely used in the field of air pollution studies. Despite well known limits, the K-closure is largely used in several atmospheric conditions because it describes the diffusive transport in an Eulerian framework where almost all measurements are Eulerian in character, it produces results that agree with experimental data as well as any more complex model, and it is not computationally expensive as higher order closures are.

The advection-diffusion equation has been widely applied in operational atmospheric dispersion models to predict ground-level concentrations due to low and tall stacks emissions. Analytical solutions of equations are of fundamental importance in understanding and describing physical phenomena, since they are able to take into account all the parameters of a problem, and investigate their influence.

In the last years (Tirabassi, 2003) special attention has been devoted to the task of searching analytical solutions for the advection-diffusion equation. Recently, the Generalized Integral Laplace Transform Technique (GILTT method) has been applied for the simulation of pollutant dispersion in the atmosphere by solving analytically the two-dimensional diffusion-advection equation assuming non-homogeneous conditions. (Moreira et al., 2006). We applied the above approach in this paper. The main steps of this method comprehend: reduction of the time-dependent problem to a stationary by the applications of the Laplace transform technique, construction of an auxiliary Sturm-Liouville problem associated to the stationary problem, expansion of the contaminant concentration in a series in terms of the obtained eigenfunctions, replacement of this expansion in the original problem. Finally, taking moment, we come out with a set of ordinary differential equations which are then solved analytically by the Laplace transform technique. The time-dependent concentration is obtained by inverting numerically the solution of the stationary problem by the Gaussian quadrature scheme.

In this work we step forward incorporating the plume rise effect (warm source) in the model using the approach proposed by Briggs (1975). A correct estimation of buoyant plume rise is one of the basic requirements for the determination of ground-level concentrations of airborne pollutant emitted by actual industrial stacks. This improvement turns out a more operative model. To investigate the influence of the plume rise effect, we report numerical simulations of the ground-level crosswind integrated centerline concentrations compared with the observed concentrations measured during the Kinkaid experiment (Hanna and Paine, 1989).

To reach this goal, we outline the paper as follows: in section 2, we report the derivation of the GILTT solution for the transient two-dimensional advection-diffusion equation. In section 3 the turbulent parameterisations assumed in this work are presented. In section 4, the plume rise approach is presented. The numerical results attained by the analytical method are reported as well the comparison with experimental data are presented in section 5, and finally in section 6, the conclusions.

2. The GILTT method

Let us consider the crosswind integrated time dependent advection-diffusion equation with advection in the x direction (as usual, the along-wind diffusion is neglected because considered little in respect to the advection):

$$\frac{\partial c(x,z,t)}{\partial t} + U\,\frac{\partial c(x,z,t)}{\partial x} = \frac{\partial}{\partial z}\left(K_z\,\frac{\partial c(x,z,t)}{\partial z}\right) , \tag{1}$$

where c denotes the crosswind integrated concentration, K_z is the vertical eddy diffusivity and U is the component longitudinal of the wind speed. Equation (1) is subjected to the boundary conditions of zero flux at the ground and PBL top, and a source with emission rate Q at height H_s:

$$K_z\,\frac{\partial c(x,z,t)}{\partial z} = 0 \qquad \text{at } z = 0,\ z = h \tag{1a}$$

$$U c(0,z,t) = Q\,\delta(z - H_s) \qquad \text{at } x = 0 \tag{1b}$$

and also assume that at the beginning of the pollutant releasing the dispersion region is not polluted, we mean:

$$c(x,z,0) = 0 \qquad \text{at } t = 0 , \tag{1c}$$

where h is the PBL height. In the sequel we consider that K_z, the wind speed U depend only on the variable z.

Using the Laplace Transform technique, transforming t into s and c into C, we have:

$$U\,\frac{\partial C(x,z,s)}{\partial x} = K_z\,\frac{\partial^2 C(x,z,s)}{\partial z^2} + K_z'\,\frac{\partial C(x,z,s)}{\partial z} - sC(x,z,s) \ . \tag{2}$$

Now we are in position to solve the stationary problem (2) by the GILTT approach. Firstly, we expand the pollutant concentration in the series:

$$C(x,z,r) = \sum_{i=0}^{N} \bar{c}_i(x,r)\zeta_i(z) \ , \tag{3}$$

where $\zeta_i(z)$ and λ_i are the respective eigenfunctions ($\zeta_i(z) = \cos(\lambda_i z)$) and eigenvalues ($\lambda_i = \frac{i\pi}{h}$ for $i = 0, 1, 2, 3, ...$) of a associated Sturm-Liouville problem. Following the procedure addopted in Wortmann et al. (2005) and Moreira et al. (2005), we replace the above ansatz in Eq. (2) and by taking moments we get:

$$\sum_{i=0}^{N}\left[\bar{c}_i'(x,r)\int_0^h U\,\zeta_i(z)\zeta_j(z)dz + \lambda_i^2\,\bar{c}_i(x,r)\int_0^h K_z\zeta_i(z)\zeta_j(z)\,dz - \bar{c}_i(x,r)\int_0^h K_z'\,\zeta_i'(z)\zeta_j(z)\,dz + r\,\bar{c}_i(x,r)\int_0^h \zeta_i(z)\zeta_j(z)\,dz\right] = 0 \ . \tag{4}$$

Rewriting Eq. (4) in matrix fashion, we obtain:

$$Y'(x,r) + FY(x,r) = 0 \ , \tag{5}$$

where $Y(x,r)$ is the column vector whose components are $\bar{c}_i(x,r)$ and the matrix F is defined like $F = B^{-1}E$. The matrices B and E are respectively given by:

$$b_{i,j} = \int_0^h U\ \zeta_i(z)\zeta_j(z)dz \tag{6a}$$

and

$$e_{i,j} = -\int_0^h K'_z\zeta'_i(z)\zeta_j(z)dz + \lambda_i^2\int_0^h K_z\zeta_i(z)\zeta_j(z)dz + r\int_0^h \zeta_i(z)\zeta_j(z)dz \,. \tag{6b}$$

The transformed problem represented by the Eq. (5) is solved by the Laplace Transform technique and diagonalization and his solution is (Wortmann et al., 2005; Moreira et al., 2005):

$$Y(x,r) = X.G(x,r).\xi \quad , \tag{7}$$

where ξ is the integration constant vector, G is the diagonal matrix with elements have the form $e^{-d_i x}$, X is the eigenfunction matrix and d_i are the eigenvalues of the matrix F. Therefore, the transformed solution given by Eq. (3) is well determined.

Finally, the time dependent concentration is obtained by inverting numerically the transformed concentration $C(x,z,r)$ by a Gaussian Quadrature scheme:

$$c(x,z,t) = \sum_{k=1}^{M}\frac{P_k}{t}A_k\sum_{i=0}^{N}\bar{c}_i(x,\frac{P_k}{t})\zeta_i(z) \tag{8}$$

where A_k and P_k are the weights and roots of the Gaussian quadrature integration scheme and are tabulated in the book by Stroud and Secrest (1966).

It is important to recall that the solution of problem (1) given by equation (8), is analytical, in the sense that no approximation is made along its derivation, except for the Laplace numerical inversion and round-off error. Regarding the issue of Laplace numerical inversion, it is important to mention, that this approach is exact if the transformed function is a polynomial of degree 2*M*-1 in the 1/*s* variable. Furthermore, we must point out that we specialize this application, without loss of generality for an eddy diffusivity coeficient depending only on the *z* variable.

3. Turbulent Parameterizations

In the atmospheric diffusion problems the choice of a turbulent parameterization represents a fundamental decision for the pollutants dispersion modeling. From a physical point of view the turbulence parameterization is an approximation to the nature in the sense that we are putting in mathematical models an approximated relation that in principle can be used as a surrogate for the natural true unknown term. The reliability of each model strongly depends on the way as turbulent parameters are calculated and related to the current understanding of the PBL (Mangia *et al.*, 2002).

The lateral dispersion parameter σ_y is important to calculate the concentration in the ground-level centerline concentration:

$$C(x,0,0) = \frac{c(x,0)}{\sqrt{2\pi}\sigma_y} \quad , \tag{9}$$

where in this study the ground-level cross-wind integrated concentration in the Eq. (9) is calculated employing the GILTT model (Eq. (8)).

The lateral dispersion parameter σ_y for a CBL derived by Degrazia et al. (1998) presents the following form:

$$\frac{\sigma_y^2}{z_i^2} = \frac{0.21}{\pi}\int_0^\infty sin^2\left(2.26\psi^{1/3}Xn'\right)\frac{dn'}{(1+n')^{5/3}n'^2} \quad , \tag{10}$$

where X is a nondimensional distance ($X = xw_*/Uz_i$), w_* is the convective velocity scale and z_i is the top of the PBL.

The Eq. (10) contain the unknown function ψ, the molecular dissipation of turbulent velocity is a leading destruction terms in equations for the budget of second-order moments, and according Hϕjstrup (1982), has the form:

$$\psi^{1/3} = \left[\left(1 - \frac{z}{z_i}\right)^2 \left(\frac{z}{-L}\right)^{-2/3} + 0.75 \right]^{1/2} , \tag{11}$$

where L is the length of Monin-Obukhov.

In terms of the convective scaling parameters the vertical eddy diffusivity can be formulated as (Degrazia *et al.*, 1997):

$$\frac{K_z}{w_* z_i} = 0.22 \left(\frac{z}{z_i}\right)^{1/3} \left(1 - \frac{z}{z_i}\right)^{1/3} \left[1 - \exp\left(-\frac{4z}{z_i}\right) - 0.0003 \exp\left(\frac{8z}{z_i}\right)\right] . \tag{12}$$

The wind speed profile used has been parameterized following the similarity theory of Monin-Obukhov and "OML" model (Berkowicz *et al.*, 1986):

$$U = \frac{u_*}{k}\left[\ln(z/z_0) - \Psi_m(z/L) + \Psi_m(z_0/L)\right] , \qquad \text{if } z \le z_b , \tag{13}$$

$$U = U(z_b) , \qquad \text{if } z > z_b , \tag{14}$$

where $z_b = \min\left[|L|, 0.1 z_i\right]$, and Ψ_m is a stability function given by (Paulson, 1970).

Thus, in this study we introduce the vertical eddy diffusivity (Eq. (12)) and wind profile (Eq. (13) and (14)) in the GILTT model (Eq. (8)) to calculate the ground-level crosswind integrated concentration. Finally, these crosswind integrated concentration and the lateral dispersion parameter (Eq. (10)) will be introduced into Eq. (9) to simulate the ground-level centerline concentrations of buoyant emissions released from an elevated continuous source point in an unstable PBL.

4. Plume rise

A correct estimation of buoyant plume rise is one of the basic requirements for the determination of ground level concentrations of airborne pollutant emitted by industrial stacks. In fact, maximum ground level concentration is roughly inversely proportional to the square of the final height h_e. For this reason, in many simple dispersion models, stack gases are assumed to be emitted from a virtual source located at height h_e along the vertical above the stack. The effective plume height h_e (elevation of plume centerline relative to ground level) results from the sum of stack height H_s and plume rise Δh:

$$h_e = H_s + \Delta h . \tag{15}$$

Some formula provide the plume rise as a function of the distance, but most of them provide a constant value (final plume rise) that the plume reaches at a large downwind distance. These formula contain height depending atmospheric variables normally specified at the stack outlet height.

Several studies and review works have provided semiempirical formula for evaluating Δh (e.g., Briggs, 1975; Stern, 1976; Hanna et al., 1982; and many others). Others researchers have provided more complex and comprehensive descriptions of several physical interactions between the plume and the ambient air (e.g., Golay, 1982; Netterville, 1990). Relevant and exhaustive review papers on the plume rise subject can be found in the literature, for instance, Briggs (1975) and Weil (1988). In this work, we are utilizing the formula of Briggs (1975) applied by Moreira (2000).

Briggs (1975) made a distinction between neutral and unstable conditions accounting for the effects of ambient turbulence on the plume rise. While self-generated turbulence affects the entrainment process near the source, ambient turbulence (with both small and large scale eddies) becomes important further downwind. Small scale eddies, are responsible for the increase of the plume growth rate beyond that given by self-induced turbulence. The breakup model (Briggs, 1975; Weil, 1988) assumes that plume rise finishes when ambient turbulence "breaks up" the self-generated structure of the plume, causing a vigorous mixing, and, consequently, gradually loses buoyancy and momentum and eventually level off. Thus, this process leads to an asymptotic rise. According to Briggs, the plume breakup occurs when the ambient rate of dissipation of turbulent kinetic energy, ε_a, exceeds the one of the plume ε. Large scale eddies (updrafts and downdrafts in the convective boundary layer (CBL)) may transport plume segments up and down, thereby dispersing the plume by vertical meandering and pushing some of them to the surface. When this happens, the time averaged ground level concentration is more dependent on how many times, during the averaging period, the plume touches the ground than on the height of the asymptotic rise. As a consequence, in the CBL case, the leading parameter is assumed to be the surface sensible heat flux, which plays the major role in the development of updrafts and downdrafts.

In strong convection ($z_i/|L| > 10$) the model "breaks up" has a final behavior given for:

$$\Delta h = 4.3\left(\frac{F}{Uw_*^2}\right)^{3/5} z_i^{2/5} \ , \qquad (16)$$

where the rate of ambient dissipation is assumed to be $0.1\frac{w_*^3}{z_i}$. The buoyancy parameter *F* is given for:

$$F = gV_i r_i^2 \frac{(T_i - T_a)}{T_i} \ , \qquad (17)$$

where V_i and T_i are the vertical velocity and temperature, respectively, in the exit of the chimney, T_a is the ambient temperature, *g* the acceleration of the gravity and r_i is the radius of the source. The model defines a "touchdown" for moderate convective conditions predicts the behavior of the plume for:

$$\Delta h = 1.0\left(\frac{F}{Uw_d^2}\right)\left(1 + \frac{2H_s}{\Delta h}\right)^2 \ , \qquad (18)$$

where w_d is the medium speed of the downdrafts, considered as $w_d = 0.4w_*$. The resulting equation is iteratively solved for Δh. In neutral stability, the "breaks up" model predicts the following behavior:

$$\Delta h = 1.3\frac{F}{Uu_*^2}\left(1 + \frac{H_s}{\Delta h}\right)^{2/3} \ . \qquad (19)$$

In this work, the penetration of the plume is not considered due to the boundary conditions of the K-model. Then, if the plume is completely prey, Weil (1979) suggests that the restriction geometric limit for Δh is:

$$\Delta h = 0.62(z_i - H_s) \ . \qquad (20)$$

In certain cases, Briggs (1975) recommends to use the formulae that provides the minimum plume rise; this result is "the most conservative", since it gives rise to the maximum values of concentration expected at the ground, thus limiting the risk of a possible underestimation. Then, the formulas can be summarized as it proceeds:

$$\Delta h = min(\text{Eqs. 16, 18, 19, 20}) \ . \qquad (21)$$

5. Experimental data and Results

The performance of the GILTT model has been evaluated against experimental ground level concentration using experimental data from dispersion experiments carried out in Kinkaid, Ilinois, USA. The Kincaid field campaign (Bowne and Londergan, 1981) concerns an elevated release in a flat farmland with some lakes. During the experiment, SF was released from 187 tall stacks and recorded on a network consisting of roughly 200 samplers positioned in arcs from 0.5 to 50 km downwind of the source. The data set includes the meteorological parameters as friction velocity, Obukhov-Monin length and height of boundary layer. The measured concentration levels is frequently irregular, with high and low concentrations occurring intermittently along same arc, moreover there are frequent gaps in the monitoring arcs. For the above reasons a variable has been assigned as a quality factor in order to indicate the degree of readability of data (Olesen, 1995). The quality indicator (from 0 to 3) has been assigned. Here, only the data with quality factor 3 were considered. A complete description of the experiment is found in the work of Hanna and Paine (1989) relatively only convective condition (for $z_i/|L| > 10$). The meteorological parameters were derived using preprocessing methods. Observed mixing heights were determined by interpretation of radiosonde data. The distributed dataset contains hourly mean values of concentrations and meteorological data. The time dependence in the model was evaluated with hourly average concentration (time resolution of 10 min) in the sampling period.

Figure 1 shows the observed and predicted scatter diagram of ground-level centerline concentrations using the GILTT model for the Kinkaid experiment. In this respect, it is important to note that the GILTT model reproduce fairly well the observed concentration.

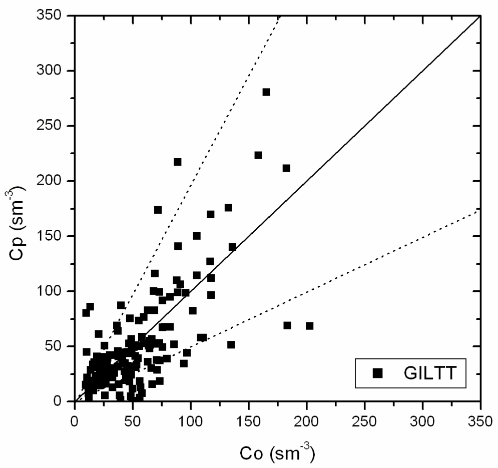

Figure 1. Observed (Co) and predicted (Cp) crosswind ground-level integrated concentration scatter diagram for the GILTT model. Dotted lines indicate a factor of two.

The datasets were applied subsequently to the following statistical indices (Hanna, 1989):

NMSE (normalized mean square error) = $\overline{(C_o - C_p)^2} / \overline{C_o}\,\overline{C_p}$,

FA2 = fraction of data (%) for $0.5 \le (C_p / C_o) \le 2$

R (correlation coefficient) = $\overline{(C_o - \overline{C_o})(C_p - \overline{C_p})} / \sigma_o \sigma_p$,

FB (fractional bias) = $\overline{C_o} - \overline{C_p} / 0.5(\overline{C_o} + \overline{C_p})$,

FS (fractional standard deviations) = $(\sigma_o - \sigma_p) / 0.5(\sigma_o + \sigma_p)$

where subscripts *o* and *p* refer to observed and predicted quantities, respectively, σ the standard deviation and an overbar indicates an average.

The results of the statistical indices for the GILTT model are compared with those obtained from a Gaussian model (Moreira et al., 2004) and are shown in Tab. 1. The statistical indices point out that a good agreement is obtained between the Gaussian and GILTT model, although the statistical indices indicate that the GILTT reproduces more adequately the observed ground-level centerline concentrations (in particular fit the Kinkaid data set, where data are more numerous and difficult to be model by dispersion models).

Table 1. Results of statistical indices used to evaluate the model performance.

Model	NMSE	R	FA2	FB	FS
GILTT	0.40	0.69	0.75	0.05	-0.22
Gaussian	0.54	0.61	0.74	0.33	0.20

6. Conclusion

In this work we present numerical simulations of pollutants diffusion released from a buoyant source, by the GILTT model. In the model we consider the dispersion parameters and eddy diffusivities described in terms of the energy-containing eddies.

The statistical analysis of the results shows a good agreement between the results of the proposed approach with the experimental data of the Kinkaid experiment and the Gaussian results. We promptly realize also that the GILTT might yield better results than Gaussian (that shows good results either) approach. Bearing in mind that in Gaussian model the turbulence is assumed homogeneous and constant dispersion parameters, we are confident that this fact explains the better performance of the GILTT model. Indeed, in the GILTT approach we consider the parameterization derived by Degrazia et al. (1997, 1998) for nonhomogeneous turbulence having a dependence on the vertical distance z. Now, we would like to stress that from above discussion, the GILTT model is a robust method, under computational point of view, to simulate the pollutant dispersion in the PBL. This argument is reinforced by the comparable computation effort between the GILTT and Gaussian solutions besides their analytical features. Finally, we will focus our future attention in the solution of the GILTT incorporating simple chemical pollutant reactions as source term, in order to make this solution an operational model to air quality simulation.

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